# Pentanamide, N-(3-nitrophenyl)-

**Inchi:** InChI=1S/C11H14N2O3/c1-2-3-7-11(14)12-9-5-4-6-10(8-9)13(15)16/h4-6,8H,2-3,7H2,1H
**InchiKey:** UYUWKCAOJYPGIZ-UHFFFAOYSA-N
**Formula:** C11H14N2O3
**SMILES:** CCCCC(=O)Nc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 222.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 140.54 | kJ/mol | Joback Method |
| hf | -115.18 | kJ/mol | Joback Method |
| hfus | 35.96 | kJ/mol | Joback Method |
| hvap | 72.79 | kJ/mol | Joback Method |
| log10ws | -3.58 | | Crippen Method |
| logp | 2.723 | | Crippen Method |
| mcvol | 171.060 | ml/mol | McGowan Method |
| pc | 2859.68 | kPa | Joback Method |
| rinpol | 2073.00 | | NIST Webbook |
| tb | 738.62 | K | Joback Method |
| tc | 972.33 | K | Joback Method |
| tf | 498.87 | K | Joback Method |
| vc | 0.666 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 470.40 | J/mol×K | 738.62 | Joback Method |
| cpg | 482.91 | J/mol×K | 777.57 | Joback Method |
| cpg | 494.45 | J/mol×K | 816.52 | Joback Method |
| cpg | 505.08 | J/mol×K | 855.48 | Joback Method |
| cpg | 514.85 | J/mol×K | 894.43 | Joback Method |
| cpg | 523.81 | J/mol×K | 933.38 | Joback Method |
| cpg | 532.01 | J/mol×K | 972.33 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U306896&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |